Dynamical Solutions to the Ground State of a Frustrated Magnet*

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Abstract: In this project, we will explore an innovative approach to simulating frustrated magnets by incorporating non-linearity to the system through the use of a mean-field approximation. Drawing inspiration from the Gross-Pitaevskii equation, which effectively models Bose-Einstein condensates via a mean-field approximation,[1] we aim to apply a similar technique to frustrated magnets in hopes of capturing their true ground state behavior more accurately. Our goal is to develop a method that can be implemented with a classical computer. If the results are promising, these methods could then be extended to quantum computer simulations, significantly expanding[2] the scale and complexity of the systems that can be modeled.

Frustrated magnet systems have garnered significant interest due to the complex and unique phenomena they exhibit.[3] These systems present considerable challenges for classical simulation methods, particularly in approximating and identifying their true ground states. The difficulty arises from the vast number of spin configurations with similar energies, making it challenging to pinpoint the actual minimum-energy state.[3]

Frustration in magnetic systems typically arises when the spins cannot satisfy all their pairwise interactions simultaneously, resulting in a highly degenerate ground state.[4] Geometric frustration is a type of magnetic frustration, caused by the spatial arrangement of particles in the lattice of the substance.[3] A classic example of this is shown with an anti-ferromagnet on a triangular lattice,[2] where each spin is coupled to two others. In this configuration, neighboring spins aim to align anti-parallel, but the triangular geometry makes it impossible for all pairs to achieve this simultaneously, leading to conflicting interactions.[2] As a result, the spins are "frustrated", and the system fails to settle into a simple ordered state.[2]

Magnetic frustration is not limited to geometric constraints; it can also arise through exchange frustration.[3] This form of frustration occurs when competing interactions between spins occur at different distances. For example, next-nearest-neighbor interactions may conflict with nearest-neighbor interactions, creating competing magnetic alignments.[3] These long-range competing interactions cause frustration even in systems with simpler lattice structures, further complicating the system's ability to find a stable ground state.

The Gross-Pitaevskii equation, commonly used to describe the dynamics of Bose-Einstein condensates introduces non-linearity through a mean-field approximation.[1] This technique allows for the efficient treatment of many-body interactions by averaging the contributions of particles in certain regions and treating them as a single particle.[1] Applying a similar concept to frustrated magnets, we hypothesize that introducing non-linearity at the boundaries could guide the system toward an approximation of its true ground state.

Our proposed methodology to investigate this hypothesis involves developing a simulation of a small frustrated magnet system. We will then introduce non-linearity at the system's boundaries using a mean-field approximation, averaging the spin values at the edges while treating the central spins as exact. This technique aims to reduce boundary discrepancies, which often lead to cumulative errors in conventional simulation methods. The ground states for small systems will then be obtained exactly by numerically diagonalizing the Hamiltonian.

The incorporation of non-linearity to the systems shows promise as a potential pathway toward more accurate and computationally efficient simulations, which can be extended to quantum computing platforms for larger systems. Our work lays the foundation for future research into optimizing simulation techniques for condensed matter physics, with potential applications in the study of exotic magnetic phenomena and quantum materials.

[*] Physical Review A (PRA) Journal Style

[1] L. Pitaevskii and S. Stringari, *Bose-Einstein Condensation* (Clarendon Press, 2003).
[2] J. Zhang, M. Yung, R. Laflamme, A. Aspuru-Guzik, and J. Baugh, Nature Communications **3** (2012).
[3] C. Lacroix, P. Mendels, and F. Mila, *Introduction to Frustrated Magnetism* (Springer Science & Business Media, 2011).
[4] C. L. Henley, Annual Review of Condensed Matter Physics **1** (2010).